

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1560 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.01e-01

Confidence level: 6.59e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Dodecanol</div> <div>Measured: 3310</div> <div>Predicted: 2560</div>	<div>Image not found</div> <div>1-Decanol</div> <div>Measured: 389</div> <div>Predicted: 347</div>	<div>Image not found</div> <div>4-Nonylphenol</div> <div>Measured: 6920</div> <div>Predicted: 1660</div>
<div>Image not found</div> <div>Ethyl octanoate</div> <div>Measured: 1050</div> <div>Predicted: 617</div>	<div>Image not found</div> <div>Pentanochlor</div> <div>Measured: 575</div> <div>Predicted: 365</div>	